Augmented Plane-Wave Method for Photonic Band-Gap Structures

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The first successfully predicted structure to yield a photonic band-gap (PBG) was that of dielectric spheres arranged in a diamond lattice.[1] Since then, there has been considerable effort to elaborate a process for the manufacturing of diamond (or diamond-like) structures at submicron wavelengths. One such approach consists in etching a large number of hole triplets at off-vertical angles in a slab.[2] Another consists in building an orderly stacking of dielectric rods.[3] Yet another consists in etching a series of horizontal grooves into sequentially-grown layers, and etching vertical holes.[4] All these structures are variations of the same diamond structure, aligned along either the (1,1,1), (0,0,1), or (1,1,0) directions, respectively. In theoretical treatments, the use of the plane-wave expansion method is common.[5,6,7] However, the simpler structures have geometries that may be amenable to special theoretical treatment.

We have developed a two-dimensional code (extendible to three dimensions) based on the Augmented Plane-Wave (APW) method of Slater[8] which is capable of band structure computations for arrays of either dielectric or conducting elements. This method allows a functional basis set that is specialized to the cylindrical geometry under study. Until this work, the plane-wave method[7] has been used for dielectrics and Rayleigh scattering theory[9] has been used for conductors.

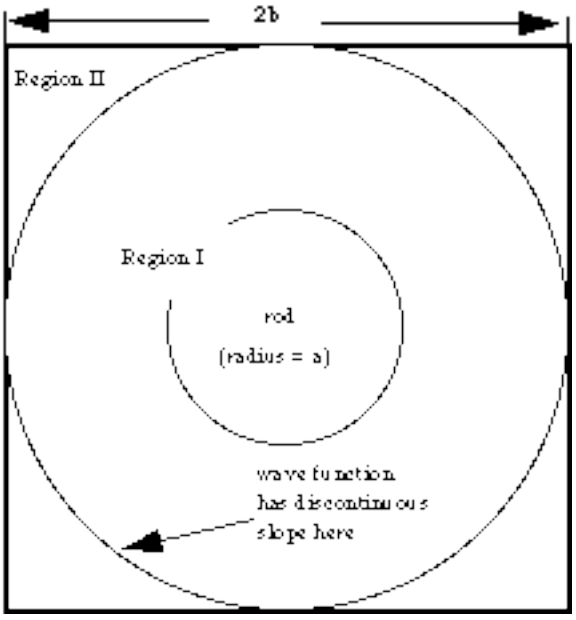

Figure 1. Wigner-Seitz cell used in calculation.

For electronic systems, the APW method is discussed several in places[10,11] in the literature; however, in general these discussions are limited to three-dimensional spherically-symmetric systems with scalar boundary conditions. Here, the use of a two-dimensional unit cell along with decomposition of the wave into two different polarization effectively changes the vector boundary conditions to scalar boundary conditions. We have chosen to use Bessel functions since they are well suited for elements with cylindrical surfaces. The result is that the form of the matrix element is only slightly different for the two dimensional electromagnetic-wave case versus the three-dimensional Schröedinger-wave case. The Wigner-Seitz cell for the two dimensional calculation is shown in Figure 1. The basis is the set of functions ψ_i, i = 1, 2, . . . n. In Region I the Bessel functions $J_m(x)$ and $Y_m(x)$ are used as the basis. In Region II free waves are used. The joining of the Bessel functions with free waves is made possible through the use of the Laurent series:

$$(1) \qquad e^{ik\cdot x} = \sum_{m=-\infty}^{\infty} i^m J_m(|k|x)\, e^{im(\varphi-\varphi_k)}$$

The joining is continuous in value, but discontinuous in derivative, at the interface. The electromagnetic wave equation with periodic boundary conditions is converted into a variational problem, which leads to the non-linear eigenvalue problem det M = 0, where the matrix elements M^{ij} are:

$$(2) \qquad M^{ij} = H^{ij} + S^{ij} - \lambda \Delta^{ij} \qquad \text{where} \qquad (3) \qquad H^{ij} = \int \psi_i^* \, H \, \psi_j \, d\Omega$$

$$(4) \qquad \Delta^{ij} = \int \psi_i^* \, \psi_j \, d\Omega \qquad \text{and} \qquad (5) \qquad S^{ij} = -\int \psi_i^* \left[\frac{\partial \psi_{j,II}}{\partial r} - \frac{\partial \psi_{j,I}}{\partial r} \right] ds$$

In the first two integrals the domain Ω is the area Region I + Region II. In the first integral the Hamiltonian operator $H = -\nabla^2 + [1 - \varepsilon(r)]$ where ε is the dielectric function. The third integral is a line integral on a contour around the circle of discontinuity. Within the integrand is the difference in the derivative of a basis function (here, with index j) between the inside and the outside of the circle. When the basis functions are inserted into the above equations the matrix elements become:

$$(6) \qquad M^{ij} =$$

$$4b^2(k_j^2 - \lambda)\delta_{ij}^2 - 2\pi b^2 (k_i \cdot k_j - \lambda) \frac{J_1(\Delta k b)}{\Delta k b} \cdot 2\pi b \sum_m J_m(k_i b) J_m(k_j b) \frac{R'_m(\sqrt{\lambda} b)}{R_m(\sqrt{\lambda} b)} \cos(m\Delta\varphi)$$

where $R_m(x) = b_m J_m(x) + c_m Y_m(x)$ and $R'_m(x)$ is the derivative of $R_m(x)$. The eigenvalue λ appears explicitly in a non-linear manner. The quantities $\Delta k = |k_j - k_i|$ and $\Delta\varphi = \varphi_j - \varphi_i$. The symbol δ_{ij} represents Kronecker's delta function.

The coefficients b_m and c_m are chosen to satisfy the boundary conditions within Region I. The boundary conditions depend on the rod material and the polarization, where in "s" polarization the electric field is parallel to the rod axis and in "p" polarization the magnetic field is parallel to the rod axis. For example, if the rod is a perfect conductor, in s polarization the field is zero at the surface of the rod and in p polarization the derivative of the field is zero. For a dielectric rod and s polarization, the electric field is continuous at the surface. For p polarization, the magnetic field is continuous. For loss-less isotropic media the matrix is real and symmetric.

The expression (6) is processed with a root finder and the roots are found as a function of the initial orientation of the propagation vector to the rod lattice. For a given value of the eigenvalue $\lambda = (\omega/c)^2$ the determinant of the matrix is found as the product of the diagonal elements in the matrix U, which is in turn obtained by LU decomposition of the matrix. These roots represent frequencies for transmission through the structure. This is analogous to finding the allowed energies for electrons in a crystal using the "electronic" APW method. One complication with this method is that poles in the determinant sometimes fall near a root. Some care must be taken in the procedure so as to not skip over those roots.

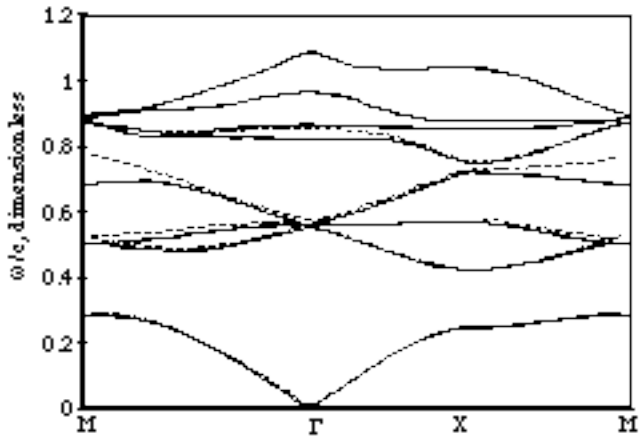

Fig. 2. Photonic s-band structure of a square lattice of rods ($\sqrt{\varepsilon}$ = 3.4) of radius 0.2 in a cell of unit dimension. The dashed and solid heavy lines are for an APW calculation with 2 and 9 basis functions, respectively. Also shown is a plane-wave calculation as a light solid line. The light line is in general hidden by the heavy solid line.

We chose to study the band diagram for an infinite array of long rods arranged on a square lattice, and compare our results with other computational methods. In the examples below, the rods are either made of dielectric material or perfect metal. In Fig. 2 s-wave results from the code described above has been compared to the plane wave method developed at MIT.[12] A square lattice of rods was chosen with a lattice constant 2b = 1.0. The dielectric rod radius was set at a = 0.20, with an index of refraction of the material of 3.40. The APW code was run with a 2x2, 4x4, 9x9 and 25x25 determinant. Comparison between the three shows that the 9x9 matrix was sufficient for convergence in this problem. It is seen that the two codes are in essentially exact agreement in this case, except only 9 basis functions were required for the APW method, versus 128 for the plane-wave method.

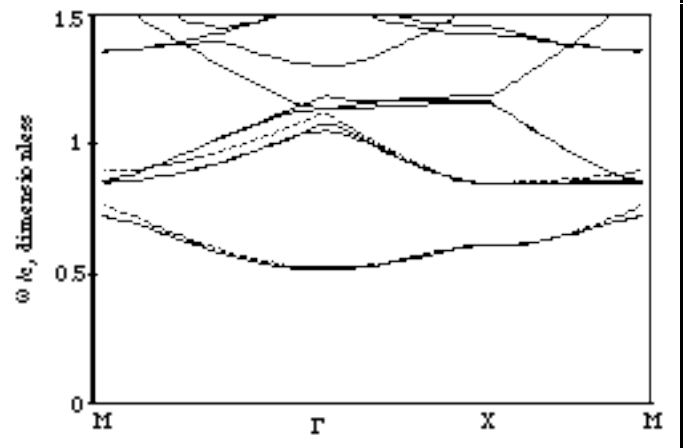

Fig. 3. Photonic s-band structure of a square lattice of conducting rods (to be compared to Figure 6 of Reference 9). The cylinder radius is 0.187. The light dotted line is the result for a 2x2 matrix. A 4x4 matrix calculation is shown as a light line. The heaviest line is the result of a 9x9 calculation.

In Figure 3 s-wave calculations for a square lattice of conducting rods is shown. The rod radius is 0.187, giving a filling fraction in the lattice of 0.11. This example was taken from Figure 6 of Reference 9. Shown are the results for a 2x2 matrix, a 4x4 matrix and a 9x9 matrix. The authors of Ref. 9 arrive at this (9x9) level of convergence with a 49x49 matrix, using their Rayleigh scattering method, which is not tremendously different from the APW method in the case of conductors. The superior convergence of the APW method is likely due to the continuous joining of functions at the Region I/ Region II interface of Figure 1, which may form a more physical basis set.

The code can be modified for three-dimensional applications. For example, a second or third plane of rods can be added in orthogonal or non-orthogonal directions. If there were three planes of rods, there would be nine rods per cell, as in Reference 3. Superlattices are also easily incorporated with this method. For instance, there can be multiple rods of various types per unit cell.

The good convergence of the APW method is due to the good match between the basis set and the geometrical shape of the structure. In general, the APW method should prove to be very useful for a wide range of structures seeing that many structures have elements with cylindrical or spherical surfaces.

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